

# Comment on arXiv:1105.6233 entitled “Neutron-Inelastic-Scattering Peak by Dissipationless Mechanism in the $s_{++}$ -wave State in Iron-based Superconductors” by S. Onari and H. Kontani

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Recently, Onari and Kontani submitted a paper<sup>1</sup> which criticizes our recent theoretical study<sup>2</sup> on the neutron scattering experiment as a probe for determining the superconducting gap in the iron pnictides. In their paper, Onari and Kontani have developed a formalism in which the imaginary part of the dynamical spin susceptibility ( $\text{Im}\chi_s(\mathbf{q}, \omega)$ ) in the superconducting state can be more accurately calculated especially in the  $\omega < 2\Delta$  regime, where  $\Delta$  is the superconducting gap. In section IIIC of their paper, they mention that the conclusions of our paper are “incorrect based on inaccurate numerical calculation”. In the present Comment, we show that this in fact is not correct.

First of all, Onari and Kontani emphasize the difference of the calculation method used, but actually, a more important difference between their calculation and ours lies in the parameter values taken. The most important difference is while we take the strength of the quasiparticle damping  $\gamma_0$  to be the same between the superconducting and the normal states, as was done in Onari *et al.*’s previous study<sup>3</sup>, they now take different values for the two states :  $\gamma_0 = 20\text{meV}$  for the normal state and  $\gamma = 10\text{meV}$  for the superconducting state. The difference of the overall  $\gamma$  form between the two papers is shown in Fig. 1. The larger the difference of  $\gamma$  between the superconducting and normal states, the greater the enhancement (hump in the  $s_{++}$  or the resonance peak in  $s_{\pm}$ ) of  $\text{Im}\chi_s$  at  $\mathbf{q} \simeq (\pi, 0)$  in the superconducting state over that in the normal state, in favor of their conclusion that the hump in the  $s_{++}$  is large enough to explain the experiments while the peak in the  $s_{\pm}$  is too large, as opposed to our conclusion. We do not deny the possibility that  $\gamma$  values may be different between the two states in the actual materials, but it is important to notice that the large difference among the studies 1–3 lies here.

On the other hand, Onari and Kontani claim that our conclusion<sup>2</sup> that “the hump in the  $s_{++}$  is small for  $\Delta = 5 \sim 10\text{meV}$  compared to the case of  $\Delta = 25\text{meV}$  or larger (as was taken in Onari *et al.*’s previous paper<sup>1</sup>)” is incorrect, based on the observation that  $\text{Im}\chi_s$  in the region  $\omega < 2\Delta$  is finite, whereas it actually should be 0 in a rigorous calculation. This finiteness is in fact due to the approximation adopted in Onari *et al.*’s previous paper<sup>3</sup>. However, as shown in Fig.4 of their new paper<sup>1</sup>,

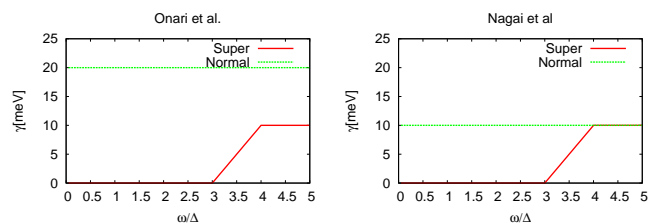


FIG. 1: The difference in the quasiparticle damping between Onari *et al.* and Nagai *et al.*.

the result of improving the  $\omega < 2\Delta$  region only results in a *suppression of the hump in the  $s_{++}$  state*. Therefore, the improvement in the  $\omega < 2\Delta$  region does not affect our conclusion regarding the enhancement around  $\omega = 2\Delta \sim 3\Delta$  in the  $s_{++}$ . As for the  $s_{\pm}$  state, we do admit that the broadness of the  $s_{\pm}$  resonance peak in Fig.1(a) of our paper may be due to the approximation, but actually we made no statement regarding this broadness, as opposed to what is mentioned in section IIIC of Onari-Kontani’s paper. In fact, we showed another calculation in Fig.1(b) of our paper<sup>2</sup> (which Onari-Kontani hardly mentions about), showing a sharper peak. As a common feature between the two cases, we mentioned only about the *height* of the peak in the  $s_{\pm}$  state with respect to that in the normal state, which is highly dependent on the strength of the quasiparticle damping in the normal state.

Also in Fig.5(a) of ref.1, they refer to our calculation result (Fig.1(a) of our paper<sup>2</sup>) and mention that the peak position of the  $s_{++}$  hump is close to  $\omega = 2\Delta$ , whereas it should be closer to  $3\Delta$ . Here, they have failed to mention the value of  $U$  in our paper, which is actually  $U = 1.375\text{eV}$ . The peak position is actually dependent on  $U$ , as already seen from the difference between  $U = 1.3\text{eV}$  and  $U = 1.32\text{eV}$  in Fig.5(a) of their paper. We have performed a calculation for several values of  $U$ , and in fact the peak position systematically varies, as shown in Fig. 2. This variance on  $U$  could be to some extent due to the approximation adopted here, but in any case, the peak position is hardly relevant to our conclusion because in Fig.1(b) of our calculation<sup>2</sup>, which Onari-

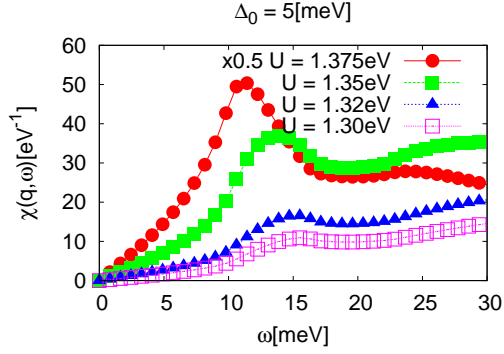


FIG. 2:  $U$ -dependence of  $\text{Im}\chi_s$  at  $\mathbf{q} = (\pi, \pi/16)$  in the  $s_{++}$ -wave state with  $\Delta = 5\text{meV}$  and  $\gamma_s = 10\text{meV}$ .

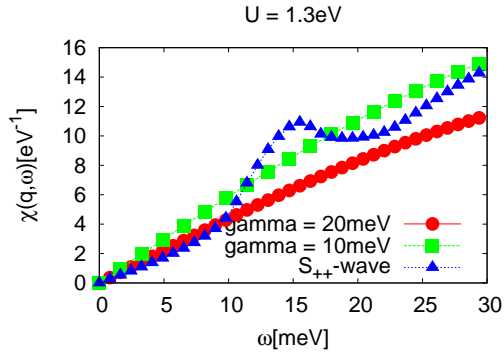


FIG. 3:  $\text{Im}\chi_s$  at  $\mathbf{q} = (\pi, \pi/16)$  with  $U = 1.3\text{eV}$ . Blue triangle is for the  $s_{++}$  state with  $\Delta = 5\text{meV}$  and  $\gamma_s = 10\text{meV}$ . Red circles and green squares are for the normal state with the damping parameter  $\gamma_0 = 10\text{meV}$  and  $20\text{meV}$ , respectively.

Kontani makes no comment on, the peak position is in fact around  $\omega = 3\Delta$ .

To further strengthen this point, we once again show in the present Comment, now adopting  $U = 1.3\text{eV}$  and  $\Delta = 5\text{meV}$ , that our conclusion holds as far as we adopt the same values of the quasiparticle damping between the normal and the superconducting states. In Fig. 3, we see that the enhancement in the  $s_{++}$  state above the normal state is small when we adopt  $\gamma = 10\text{meV}$  for both states. On the other hand, if we adopt  $\gamma = 20\text{meV}$  only for the normal state, the  $s_{++}$  hump now appears to be large, consistent with Onari-Kontani's claim. However, there does lie a quantitative difference between their calculation and ours: in the high energy regime of  $\omega = 6\Delta$  or more,  $\text{Im}\chi_s$  in the superconducting state with  $\gamma_s = 10\text{meV}$  merges to the normal state values with a different  $\gamma_0 (= 20\text{meV})$  in Onari-Kontani's calculation<sup>1</sup> (Fig.2 and Fig.3 of their paper), while in our calculation it merges to the normal state values with the same  $\gamma_0 (= 10\text{meV})$ . In the high energy regime, the effect of the superconducting gap should disappear, so that we believe our results are more physical. We are not sure about the origin of this discrepancy.

To conclude, the main difference between Onari-Kontani's calculation<sup>1</sup> and ours (especially Fig.1(b))<sup>2</sup> lies in the choice of the quasiparticle damping in the normal state, not in the method or the accuracy of the calculation. Their claim that the conclusions of our paper are "incorrect based on inaccurate numerical calculation" has no basis and is in fact not correct. If we consider the possibility of the  $\gamma$  values being different between the superconducting and the normal states (which we do not deny), then the ambiguity of determining the superconducting gap form solely from the neutron scattering at  $\sim (\pi, 0)$  will be greater. Then our proposal to look into wave vectors other than  $(\pi, 0)$  will have even more important implication<sup>2</sup>.

<sup>1</sup> S. Onari and H. Kontani, arXiv:1105.6233 (unpublished).

<sup>2</sup> Y. Nagai and K. Kuroki, to be published in Phys. Rev. B. Rapid Comm., arXiv:1103.0586.

<sup>3</sup> S. Onari, H. Kontani and M. Sato, Phys. Rev. B **81**, 060504(R) (2010).